

2-Nitropropane  
79-46-9 | DTXSID6020981

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 12.6 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.41e-01

Confidence level: 7.95e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dichloroacetic acid</div> <div>Measured: 17.2</div> <div>Predicted: 2.06e-01</div>	<div>Image not found</div> <div>Dimethylaminoethanol</div> <div>Measured: 10.1</div> <div>Predicted: 2.33</div>	<div>Image not found</div> <div>2,3-Dimethylbutan-2-ol</div> <div>Measured: 12.0</div> <div>Predicted: 5.17</div>
<div>Image not found</div> <div>Methyl acetate</div> <div>Measured: 20.8</div> <div>Predicted: 198</div>	<div>Image not found</div> <div>Ether, isobutyl methyl</div> <div>Measured: 3.79</div> <div>Predicted: 201</div>	